

A repository of 3-D models of cytoskeletal proteins has been created

3D structures of macromolecular cytoskeleton protein complexes have been reproduced; mechanisms of their functioning have been studied

A system for high-throughput molecular docking and virtual screening of antimicrotubular effect has been developed

A constantly updated repository of low-molecular compounds with antimictotubular effect has been created

A methodology for verification of target protein complexes with selected active substances has been proposed

The effect of selected compounds has been tested

Fig. 1. Application of Grid VO CSLabGrid to the bio-informational study of cytoskeleton and high-throughput virtual screening of substances having antimicrotubular effect

Fig. 2. Results of control docking of N-(3,5-dimethoxyphenyl)-3-[3-(3-methoxianiline)-1H-1,2,4-triazole-5-yl] pyridine-2-amine in the GTP-exchange site of α-tubulin with *B. taurus* (PDB structure: 1I4T)

Fig. 3. GTP-exchange site of α-tubulin with *B. taurus* (PDB structure: 114T) in combination with podophyllotoxin (CHEMBL61, red) and CHEMBL409088, 2-(3-hydroxy-4-methoxyphenyl)-6-methoxy-1-benzofuran-3-yl]-(3,4,5-trimethoxyphenyl)methanone (green)

Fig. 4. Example of structural conformation comparison of leader compounds and control substance (N-(3,5-dimethoxyphenyl)-3-[3-(3-methoxyaniline)-1H-1,2,4-triazoles-5-yl] pyridine-2-amine) according to the results of docking in CCDC Gold (with α-tubulin complexes as example)